

Bicyclo[4.4.1]undeca-1,3,5-triene

Inchi:	InChI=1S/C11H14/c1-2-6-11-8-4-3-7-10(5-1)9-11/h1-2,5-6H,3-4,7-9H2
InchiKey:	POQPGBIFWKXZAJ-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	<chem>C1=CC=C2CCCCC(=C1)C2</chem>
Mol. weight [g/mol]:	146.23
CAS:	38795-15-2

Physical Properties

Property code	Value	Unit	Source
gf	188.78	kJ/mol	Joback Method
hf	35.51	kJ/mol	Joback Method
hfus	10.76	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.373		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	502.69	K	Joback Method
tc	740.24	K	Joback Method
tf	267.81	K	Joback Method
vc	0.485	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.58	J/mol×K	502.69	Joback Method
cpg	304.13	J/mol×K	542.28	Joback Method
cpg	321.38	J/mol×K	581.87	Joback Method
cpg	337.40	J/mol×K	621.46	Joback Method
cpg	352.26	J/mol×K	661.06	Joback Method
cpg	366.02	J/mol×K	700.65	Joback Method
cpg	378.75	J/mol×K	740.24	Joback Method
dvisc	0.0035581	Paxs	267.81	Joback Method
dvisc	0.0017526	Paxs	306.96	Joback Method

dvisc	0.0010133	Paxs	346.10	Joback Method
dvisc	0.0006549	Paxs	385.25	Joback Method
dvisc	0.0004587	Paxs	424.40	Joback Method
dvisc	0.0003412	Paxs	463.54	Joback Method
dvisc	0.0002658	Paxs	502.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38795152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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